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Georgetown University
Department of Chemistry

NOV 3 1987

Final Technical Report Contract F49620-84-C-0073

U.S. Air Force Office of Scientific Research For the period September 10, 1984 to September 14, 1987

An earlier comprehensive interim technical report was submitted to cover the period from September 10,1984 to June 5, 1986.

During the period covered by this report, six plenary meetings of the Chemistry Research-evaluation Panel for the Air Force Office of Scientific Research have been held. The sixty-ninth chemistry research evaluation meeting for Air Force Office of Scientific Research was held at Santa Fe, New Mexico on November 8 and 9, 1984; forty proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix I. The seventieth chemistry research-evaluation meeting for the Air Force Office of Scientific Research was held at Baltimore, Maryland on May 9 and 10, 1985; sixty-one proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix II. The seventyfirst chemistry research-evaluation meeting for the Air Force Office of Scientific Research was held at Galveston, Texas on November 14 and 15, 1985; sixty-three proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix III. The seventy-second chemistry research-evaluation meeting for the Air Force Office of

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Scientific Research was held at Alexandria, Virginia on May 15 and 16, 1986; fifty-eight proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix IV. The seventy-third research-evaluation meeting was held at The U.S. Air Force Academy, Colorado on November 13 and 14, 1986; thirty-three proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix V. The seventy-fourth chemistry research-evaluation meeting was held at Georgetown University on May 14 and 15, 1987; thirtynine proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report has been submitted and is appended as Appendix VI. During the period of this report, a total of two hundred and ninety-four proposals in the chemical and atmospheric sciences were evaluated and ranked.

Panels of evaluators were provided for contractors' meetings that dealt with specific portions of the on-going Air Force Office of Scientific Research chemistry research program. These meetings were held in Albuquerque, New Mexico in October, 1984; in Dayton, Ohio in November, 1985 and in Bedford, Massachusetts in October, 1986. Reports covering each of these meetings have been submitted.



A-1

Persons who have served as members of Chemistry and atmosphericscience evaluation panels during this period include:

Professor Claude F. Bernasconi Department of Chemistry The University of California Santa Cruz, California 95064

Dr. Enrico Clementi IBM Fellow IBM Corporation, Kingston, New York 12401

Professor Joyce Y. Corey Department of Chemistry The University of Utah Salt Lake City, Utah 84112

Dr. Joseph E. Demuth Thomas J. Watson Research Center IBM Corporation Yorktown Heights, New York 10598

Dr. Jimmie D. Doll Department of Chemistry Los Alamos National Laboratory Los Alamos, New Mexico 87545

Professor Dennis H. Evans Department of Chemistry The University of Wisconsin Madison, Wisconsin 53706

Dr. George S. Hammond
Director
Integrated Chemical Systems
Laboratory
Allied-Signal Corporation
Morristown, New Jersey 07960

Professor William B. Hanson Director Center for Space Sciences The University of Texas, Dallas Richardson, Texas 75080

Professor H. James Harwood Chairman Institute of Polymer Science University of Akron Akron, Chio 44325 Professor James Holton Department of Atmospheric Science The University of Washington Seattle, Washington 98195

J. J. Lagowski Piper Professor of Chemistry The University of Texas Austin, Texas 78712

Professor Donald Levy Chairman, Department of Chemistry The University of Chicago Chicago, Illinois 60637

Professor Robert J. Madix Department of Chemical Engineering Stanford University Stanford, California 93405

Professor C. Bradley Moore Chairman, Department of Chemistry The University of California Berkeley, California 94720

Professor Royce W. Murray Department of Chemistry The University of North Carolina Chapel Hill, North Carolina 27514

Professor Robert Silbey
Department of Chemistry
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Professor William C. Stwalley Department of Chemistry The University of Iowa Iowa City, Iowa 52242

Professor Richard P. Van Duyne Department of Chemistry Northwestern University Evanston, Illinois 60201

Dr. Field H. Winslow
Bell Laboratories
600 Mountain Avenue
Murray Hill, New Jersey 07974

Teams of evaluators were provided on several occasions to evaluate portions of the research program of the Air Force Office of Scientific Research. Teams evaluated contractors' meetings in the field of chemical dynamics held in the Fall of each of the three years covered by the contract; in October, 1984 in Albuquerque, New Mexico, in November, 1985 in Dayton, Ohio and in November, 1986 in Concord, Massachusetts. Interim technical reports have been submitted to cover these activities.

A special research-evaluation panel was constituted for the purpose of advising the Director of Chemical Sciences, Air Force Office of Scientific Research, and other appropriate Air Force officers and civilian scientific officers concerning a program in high-energy-density materials being conducted by the Air Force Rocket Propulsion Laboratory. Two meetings were organized at which contractors and prospective contractors presented discussions of their scientific work, one in Washington, DC, March 20-21, 1986 and on in Rossyln, Va. on May 12 and 13, 1987. In connection with each of these contractor's meetings, and also in Lancaster, California on May 17 and 28, 1986 and at The U.S. Air Force Academy, Colorado on November 12 and 13, 1986 meetings of the high-energy-density-materials research-eveluation panel were held to consider proposals and to provide other evaluation of the high-energy-density program. A total of fifty-seven proposals was considered at these three meetings, and relative rankings for scientific quality were determined. Reports were submitted to cover these activities. An evaluation team was constituted to evaluate certain research being carried out at the California Institute of Technology. A report of findings of that evaluation was submitted. (Appendix VII)

Persons who have been members of the high-energy-density materials panel are:

Professor Charles F. Bender Advanced Computational Methods Center The University of Georgia Athens, Georgia 30602

Professor William Happer Department of Physics Princeton University Princeton, New Jersey 08544

Professor M. Frederick Hawthorne Department of Chemistry The University of California Los Angeles, California 90024

Dr. Ronald R. Herm The Aerospace Corporation Los Angeles, California 90009

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Submitted by,

Dr. Marilyn E. Jacox Molecular Spectroscopy Division The National Bureau of Standards Gaithersburg, Maryland 20899

Lewis H. Nosanow Vice Chancellor for Research The University of California Irvine, California 92717

Professor Isaac F. Silvera Lyman Laboratory of Physics Harvard University Cambridge, Massachusetts 02138

Professor William C. Stwalley Iowa Laser Facility The University of Iowa Iowa City, Iowa 52242

Joseph E. Earley

Principal Investigator October 26, 1987

Georgetown University

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Department of Chemistry

Revised Technical Report for AFOSR Chemistry Research-Evaluation

| | Category I | | Category II | | |
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| | 78 | DeLevie* | 71 | Redner | |
| | | | 74 | Heaven | |
| | | | 65 | Cool | |
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| A-/B+ | | | 69 | Thompson | |
| · | | | 67 | Gardner | |
| B+ | 66 | Weber | 68 | Wolf | |
| | 81 | Horn | 63 | Liu/Ziv/Tsong | |
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| | 78 | DeLevie | 98 | Mukamel** | |
| | 99 | SELLA / Francks | | | |

| 78 | DeLevie |
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| 88 | White/Kyu** |

not ranked in conjunction with other A's additional review required

Joseph E. Barley Professor and Chairman Principal Investigator December 5, 1984

Georgetown University

Department of Chemistry

Contract F49670-84-C-0073

Interim Technical Report for AFOSR Chemistry Research-Evaluation

| | Cate | egory I | | | Cate | gory II |
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^{*}additional review suggested

Joseph E. Earley Professor and Chairman Principal Investigator May 15, 1985

Georgetown University Department of Chemistry

Interim Technical Report for AFOSR Chemistry Research-Evaluation

| | Categ | gory I | Cate | egory II | Cat | egory III |
|----|-------|-----------------|------|----------------------|-----|-----------|
| A | 103 | Stone | 83 | Yates | 62 | Tsunoda |
| A | 104 | McCreery | 76 | _ | 73 | Wickwar |
| | 204 | | 77 | Goddard | 71 | McClure |
| A- | 109 | Ratner | 92 | Hemminger | 64 | Markson |
| | 90 | Geoffroy | | Leventhal | 69 | Imhof |
| | 91 | Davis | | McKoy | 63 | Dunkerton |
| | 111 | | | Engel | | |
| | 117 | Gillis(*) | | Martin | | |
| | 94 | Lemal | - | Erskine | | |
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| | 72 | Welch | 82 | Ogilby | | |
| | 80 | Caruso | 67 | | | |
| | 106 | Isayev* | 89 | Davis (therm) | | |
| | | - | 125 | | | |
| | | | 99 | Jones & Weatherford* | | |
| | | | 87 | Hopster* | | |
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| | | | 118 | Helvajian | | |
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| С | 95 | Kordas | 81 | McQuistan | 66 | Ganguly |
| - | 105 | Brostow | | | | |
| | 110 | Neelakantaswamy | | | | |

Joseph E. Earley Professor and Chairman Principal Investigator November 18, 1985 *tentative ranking, pending furthur rev

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Georgetown University Department of Chemistry

Interim Technical Report for AFOSR Chemistry Research-Evaluation Contract F49620-84-C-0073

| | Category I | Category II | Category III |
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| С | 31 Deymier | | 130 Armstrong |

Joseph E. Earley Professor and Chairman Principal Investigator May 20, 1986

*in both I and II

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Georgetown University Department of Chemistry

Interim Technical Report for AFOSR Chemistry Research-Evaluation Contract F49620-84-C-0073

| | Category I | Category II | Category III | Category IV |
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| A+ | | | • | 344 Moore 345 Lester |
| A | 70 Ratner 82 Schrock | 86 Neumark 80 Prasad* | 60 Hernandez | 314 Cassasa 320 Engelking 342 Bae 305 Carpenter |
| A- | 65 Doherty 71 Ellis 80 Prasad* | 55 Mukamel 73 Williams 56 Fano 77 Kolb 81 Guberman | | 302 Bernath 341 Daley 338 Schaeffer 340 Scobilgen 325 Weitz 319 Apkarian |
| B+ | 64 Holmes 83 Hosmane 74 Damrauer 72 Lagow 59 Norman 78 Wolfe | 79 Rabitz# 54 Bauer 75 Leventhal 66 Page 88 Coombe 84 Fenn | 68 Balachandran | 311 Gilbert 315 Brener 333 Dagligian 335 Kirby 336 Hardwick 306 Politzer 334 Hiller |
| В | 58 White | 76 Abeles 61 Peterson | 69 D'Angelo . 67 Pielke | 343 Nicolaides 303 Eisenthal 331 Yarkony 309 Wight 301 Shearer 313 Allen 304 Nichol |
| С | 63 Abrahamson | 57 Khait 62 Brown | | 307 Davis 308 Ortiz 316 Garrett 323 McFarlane 346 Bass 347 Kumar |
| R | 7 | | | 312 Haloulak |

Joseph E Earley
Professor and Chiarman
Principal Investigator

*in both category I and category II #additional reviews pending

November 14, 1986

Georgetown University Department of Chemistry

Interim Technical Report for AFOSR Chemistry Research-Evaluation

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| B+ | 31 Kuivila 19 King 29 Boudjouk 37 Fratini 08 Goodenough | 16 Gole 15 Bauer 39 Oldenburg | 06 Adams 36 Lee* 38 Uthe* | 207 Dagdigian 204 Steadman 212 Hehre 202 Kirby |
| В | 01 Huppert 14 Lee 34 Donahue 25 Welsh | 07 Czanderna 24 Whitehead 21 Felder 22 Turner | | 205 Hardwick 213 Eisenthal 214 Harbottle* 208 Ortiz 209 Kinkead (Matrix part) 210 Allen |
| С | 18 Mark | 30 Bates# 32 Lowdin | | 211 Vernecker |

Joseph E. Earley Professor and Chairman Principal Investigator

May 15, 1987

*tentative rating, pending further review.

*proposal insufficient and incomplete

DEPARTMENT OF THE AIR FORCE AIR FORCE ASTRONAUTICS LABORATORY (AFSC) EDVARDS AIR FORCE BASE, CALIFORNIA 93523-5000

RTAO: CX (Lt Lauderdale, 5413)

1 5 JUL 1987

SUBJ: Trip Report for Visit to the California Institute of Technology (Cal Tech) on 14 Jul 87

TO: CX CC/CV/CA IN TURN

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- 1. Abstract. On 14 Jul 87, Lt Walter Lauderdale visited Prof Aron Kuppermann at the California Institute of Technology. Accompanying him on this visit were Dr William Stwalley and Dr Ron Herm, chairman and member of the High Energy Density Matter (HEDM) technical evaluation panel, respectively. The purpose of this visit was to evaluate the technical progress and future plans of contract F04611-86-K-0076, "Experimental Studies of the Properties of Trihydrogen and Tetrahydrogen". The evaluation was prompted by three factors: 1) the seeming lack of progress in the project, 2) the high cost of the overall contract, and 3) FY88 budget constraints.
- Background. On the morning of 14 Jul 87, prior to the meeting with Prof Kuppermann, Lt Lauderdale met with Dr Herm and Dr Stwalley to discuss the history of Prof Kuppermann's work for the AFAL. Copies of all progress reports and the technical portion of the original proposals, along with the program plans were sent to them earlier. Prof Kuppermann's first contract to the AFAL was awarded in response to the original tetrahydrogen PRDA. This project set ambitious goals of performing H3* + HI crossed beam experiments to determine the possible existence of H4. During the course of the project, numerous setbacks occurred due to a large attenuation of the H3 beam intensity when the source was mated to the crossed beam chamber. The final result of the original contract was a redesigned H3 source and increased awareness of unforeseen difficulties, but no conclusive crossed beam experiments were performed (see AFRPL-TR-86-103, attached). The current contract is a continuation of this effort. During the first 11 months of the present effort, problems with H3 beam intensity have continued to plague the research. Improvements have been made incrementally and systematically over this time and have resulted in a methodology to locate and center the H3 beam. This provides the intensity, but it is still 3 orders of magnitude less than in the original H3 beam apparatus. The progress to date of the current contract is summarized in the attached quarterly report. This report was submitted as a precursor to the on-site evaluation. Dr Herm and Dr Stwalley were asked to assist in the evaluation in view of their respective backgrounds in molecular beams and in their role as members of the HEDM technical evaluation panel.

- 3. Results. Prof Kuppermann reviewed his work and was asked questions by Dr Herm and Dr Stwalley during this time. A summary of this discussion is detailed follows.
- a. The H3 beam source is initially aligned optically. However, when the arc discharge is started, the H3 beam does not follow the optical axis. Therefore, the beam never appears at the detector because it never passes through the slit aperture downstream. The beam was found by using a larger slit, but a larger slit leads to poor collimation of the beam and a low intensity in the crossed beam interaction region. The solution has been to use a diaphragm slit which can be opened wide (12 mm) to allow location of the beam. The entire source and support structure is then physically rotated around an axis which passes through the arc discharge port. This then brings the beam into the center of the diaphragm and the diaphragm is then closed down to the operating diameter (2 mm).
- b. This final solution has consumed the better part of two years (over both contracts). The reasons for this has been that Prof Kuppermann is developing a technology that is available nowhere else. While H3 has been made and characterized by several groups, no other group has a source of any metastable which is as intense as Kuppermann's (in the original H3 beam configuration). Many different variables have had a drastic affect on beam intensity and alignment. These include, but it not limited to, the pressure of the H3 arc source cooling water, the grade of titanium metal used for the anode and cathode of the arc discharge, and the intensity of the background light emitted from the arc discharge (reflected in the current solutions to avoid the light problem within the detector). The affect of these variables, for the most part, were unforeseeable. Also, since this is a unique arc source, the problems could only be discovered after many runs and an examination of the empirical evidence. These were in addition to the normal operating parameters of the experiment such as slit width, skimmer distance, H2 back pressure, discharge voltage, downstream pressure, and all aperture widths, to name a few.
- c. The collimation requirement for the beam is quite stringent. This is because the angular region of interest for the scattering experiments is within several degrees of the peak in the H3 beam intensity. If the beam is not well collimated, then its signal will mask the signal from the scattered products of the crossed beams. Closing the aperture to achieve good collimation, however, is useless if the beam does not pass through the resulting slit. This demonstrates how crucial the alignment is in this experiment. In addition, there are still some questions that should be answered about the H3 beam source itself. All of the issues are to be addressed in the H3 phase of the contract, which is scheduled to start upon completion of the H4 work.
- 4. Conclusions. Taking into consideration all the results and the discussions with Dr Herm and Dr Stwalley, conclusions are:

- a. The H3 beam source still requires characterization and refinement independent of the H4 experiment.
- b. In retrospect, the HEDM panel and the AFAL made a mistake in having Prof Kuppermann do the H4 work before the H3 work, which is reversed from the proposal. Prof Kuppermann made a mistake in agreeing to the change. Many of the problems he has run into may have been solved in the H3 work. Doing the H4 work first, however, made sense at the initiation of the contract because H4 was a highly visible part of the ARIES program.
- c. The current crossed beam chamber is antiquated. Its use forces a long H3 beam path and attenuates the intensity greatly (intensity is proportional to $1/r^2$). Also, other detection methods which are more sensitive are too large to fit within the chamber, also affecting intensity measurements.
- d. Given the current laboratory apparatus, Dr Stwalley and Dr Herm felt that Prof Kuppermann's approach to the problems has been acceptable.
- e. Dr Herm and Dr Stwalley believe that conclusive crossed beam results will not occur for at least six months. They also feel that the H4 work should be given no more than 12 months more effort.
- f. Dr Herm and Dr Stwalley both emphasize that Prof Kuppermann's work is at a level more basic than fundamental research. The technology of the intense metastable H3 beam is important scientifically. By the very nature of its development, it is difficult to predict all the problems to be surmounted.
- g. Dr Herm and Dr Stwalley believe that a well characterized H3* source is a very valuable asset to the ARIES program's search for new, novel energetic species. H3* is a very energetic reactant which could be combined with other species to yield a new, high energy density molecule.
- 5. Recommendations. The recommendations for actions regarding this contract are:
 - a. Give approval for Prof Kuppermann to begin the work on H3.
- b. Pass along suggestions from Dr Herm and Dr Stwalley on Prof Kuppermann's experimental procedures.
- c. Negotiate a modification to the contract to suspend the H4 work and place an option to continue it after the H3 work has been completed. The decision to continue the H4 work will be based on the H3 work and the H4 work (theoretical and experimental) being done by other HEDM contractors.
- d. Negotiate to delete the purchase of an additional quadrupole mass spectrometer for the H3 work (Dr Herm and Dr Stwalley feel the mass spectrometer used in the original H3 work will be sufficient for

the proposed B3 work).

- e. Discuss the possibility of stretching out the effort to ease the budgetary pressure in FY88.
- f. Adjust the HEDM FY88 budget (Cluster D-7) to reflect continuation of this contract.

WALTER J. LAUDERDALE, 1Lt, USAF Project Manager

- 2 Atch
- 1. AFRPL-TR-86-103
- 2. Progress Report

iLMD